Predictive Simulations of Particle-laden Turbulence in a Radiation Environment

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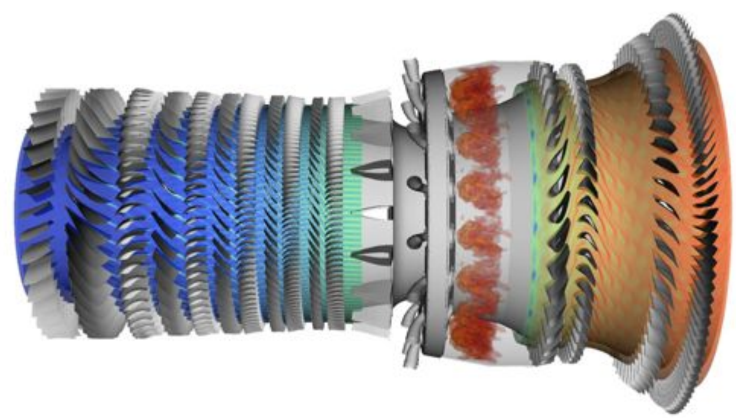
DOE/NNSA Centers of Excellence at Stanford

1997-2007 ASC Center
Advanced Simulation and Computing



Objective: end-to-end jet engine simulation

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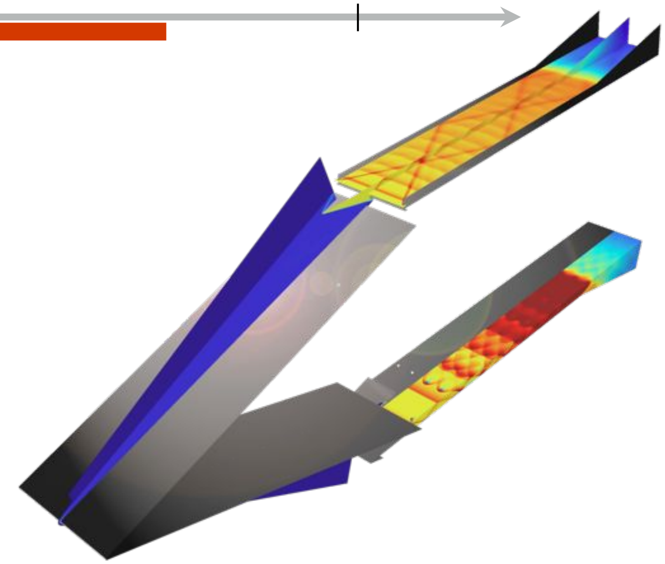
2008-2013 PSAAP Center
Predictive Science Academic Alliance Program



Objective: end-to-end hypersonic scramjet simulation

DOE/NNSA Centers of Excellence at Stanford

1997-2007 ASC Center
Advanced Simulation and Computing

2008-2013 PSAAP Center
Predictive Science Academic Alliance Program

2013-2018 PSAAP II Center

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a collaboration between

Stanford University - University of Michigan - Stony Brook University
University of Minnesota - University of Colorado - University of Texas

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Mission:

To develop and demonstrate predictive multi-physics simulations of particle-laden turbulence subject to radiation on next-generation exascale compute systems

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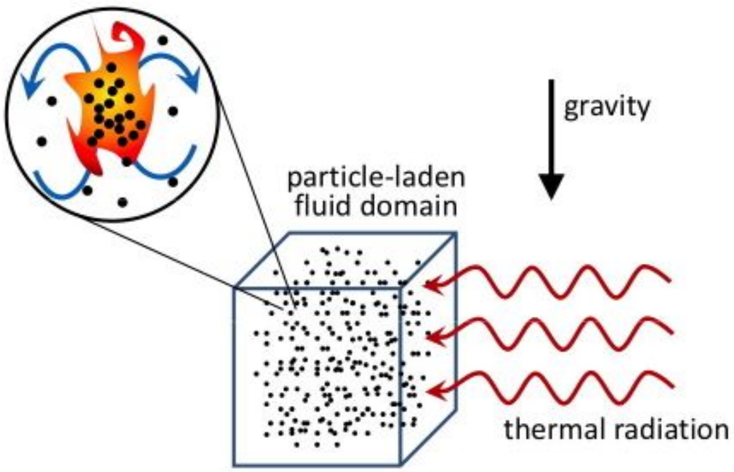
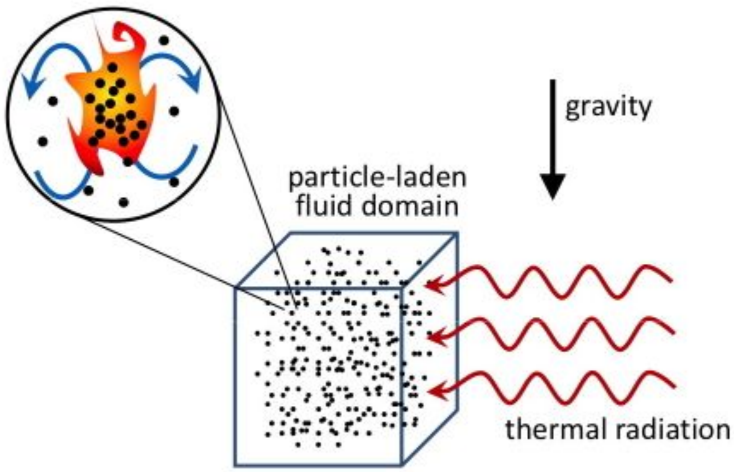
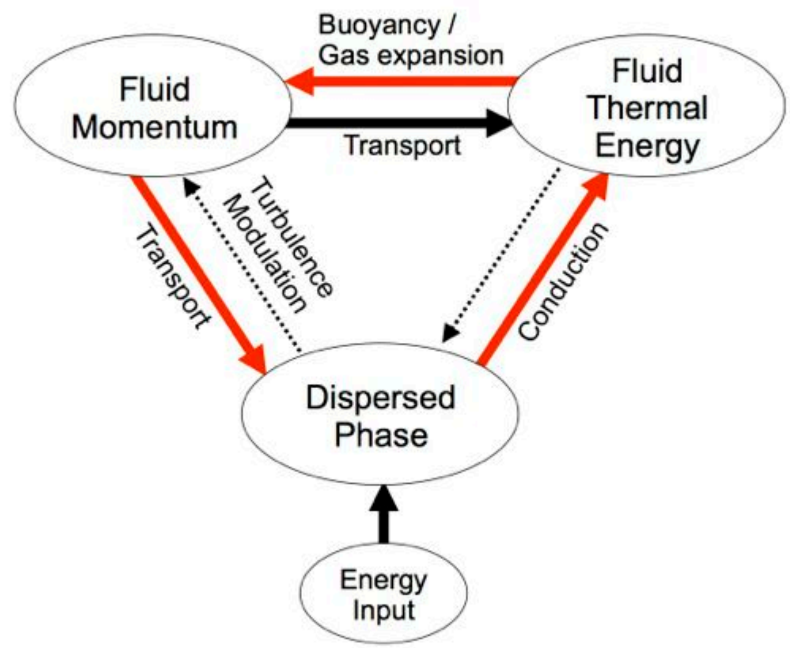
Multiphysics Scenario



In the absence of external forcing
particle-laden turbulence decays…
What happens with radiation ?

Multiphysics Scenario





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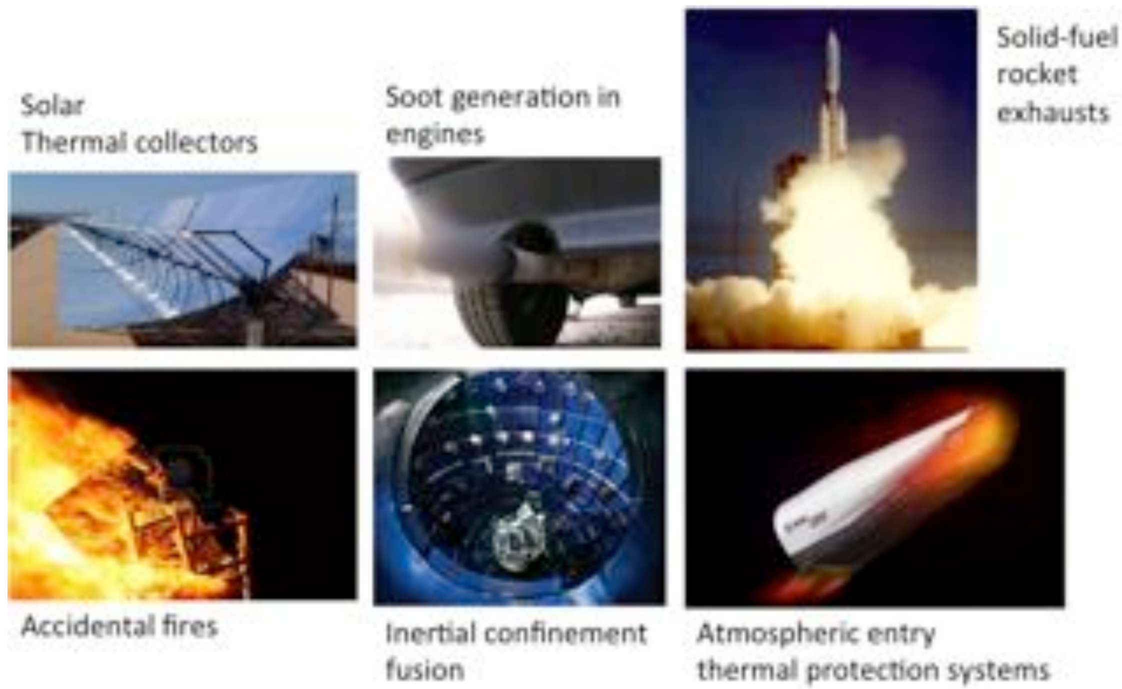
Relevant Applications



Regime of interest

Volume fraction (particle loading)

Ratio of T_{mix} and T_{source}

Shadow Fraction (opacity)

application	St	Re	Ma	ϕ	θ	SF
solar thermal collectors	0.1-10	10^5-10^6	≤ 0.3	10^{-6}-10^{-3}	0.1-0.3	≈ 1
fuel cracking	10^{-3}-10^{-1}	10^4-10^6	≤ 0.3	10^{-6}-10^{-4}	≈ 0.3	≈ 1
fuel atomization	0.01-1	10^6-10^9	≈ 0	$\approx 10^{-6}$	≈ 0	≤ 1
soot in engine combustors	$\ll 1$	10^6	≤ 1	10^{-9}-10^{-5}	≈ 1	$\ll 1$
exhaust solid-fuel rockets	$\approx 10^{-3}$	10^6	$1-4$	$\approx 10^{-8}$	≈ 1	≥ 1
ablative thermal protections	10^{-3}-10^{-1}		$7-30$	10^{-6}-10^{-4}		

[redacted]

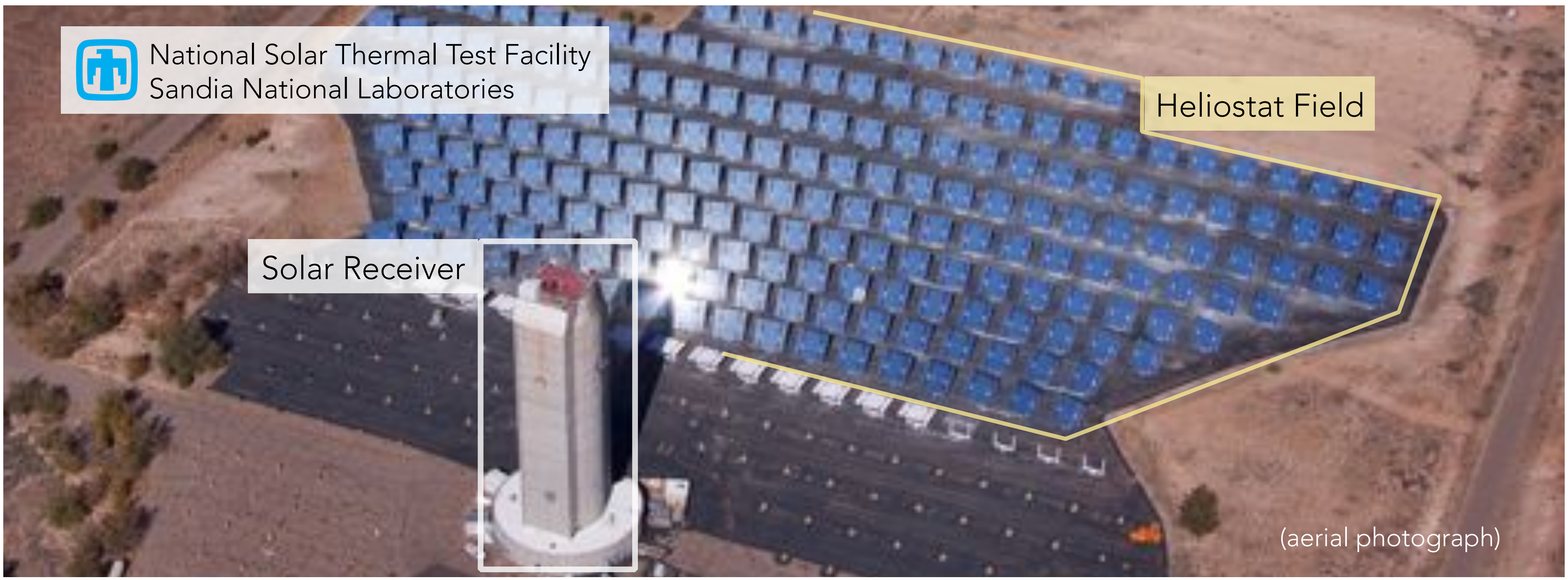
Particle Stokes #

Fluid Re #

Fluid Ma #

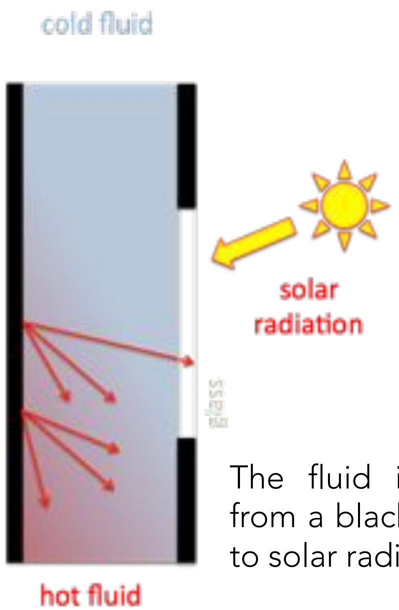
Solar Thermal Systems

Goal:
Harness and convert solar energy into thermal energy



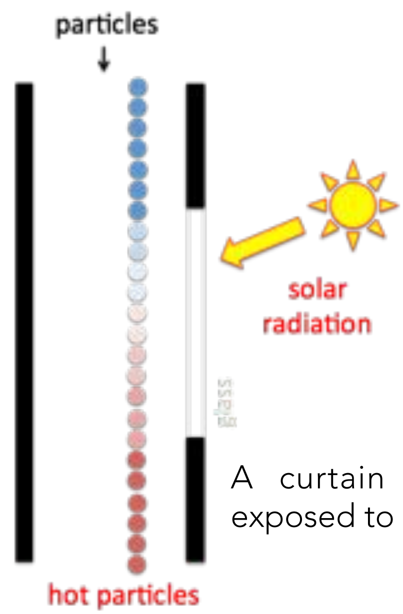
Solar Receivers

Fluid-based Receiver



The fluid is heated by conduction from a black surface which is exposed to solar radiation

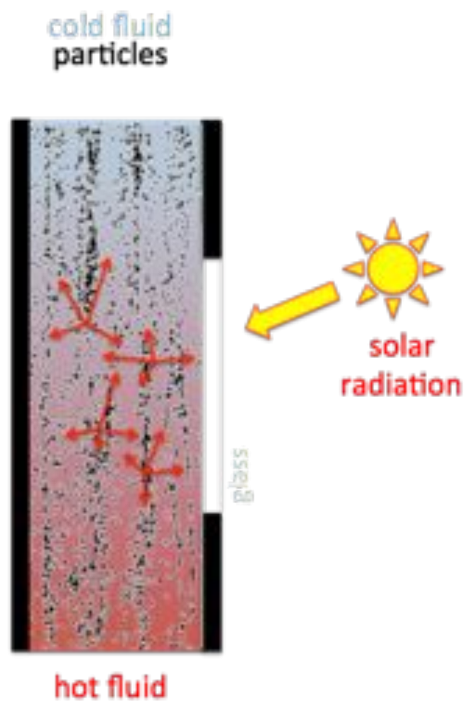
Particle Receiver



A curtain of particles is directly exposed to solar radiation

Technological Opportunity

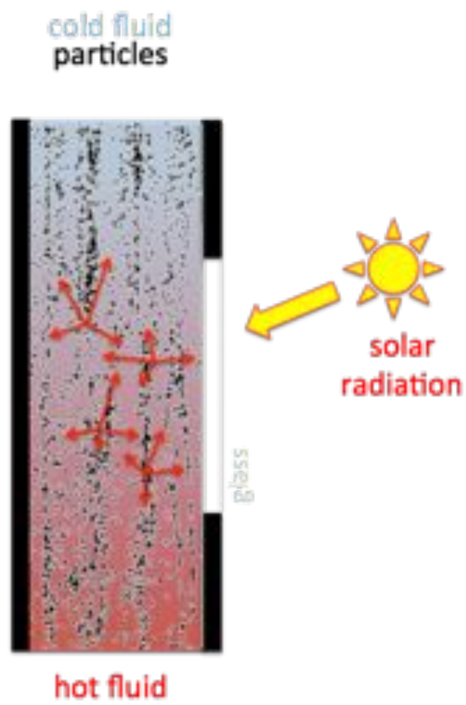
Particle-laden Flow Receiver



Moving from surface heating to volumetric heating:
Particles laden in the fluid absorb solar radiation and through conduction heat the surrounding fluid

Technological Opportunity

Particle-laden Flow Receiver



Moving from surface heating to volumetric heating:
Particles laden in the fluid absorb solar radiation and through conduction heat the surrounding fluid

Questions:
- Is this system more efficient?
- Can it be scaled for higher energy production?
- Can the particle size be adjusted to reduce the impact of solar radiation variability?

Scientific Challenge

Multi-physics coupling of: turbulence, radiation, and particle transport

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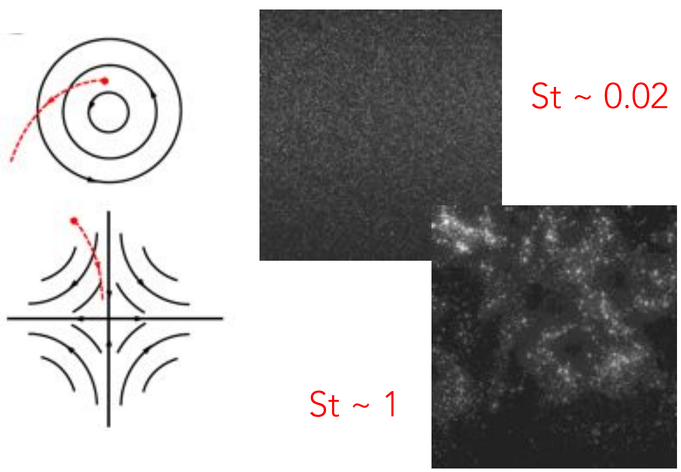
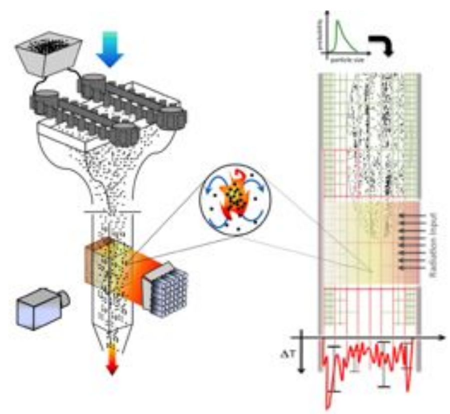
Multi-physics coupling of: turbulence, radiation, and particle transport

Starting point is particle-laden turbulence



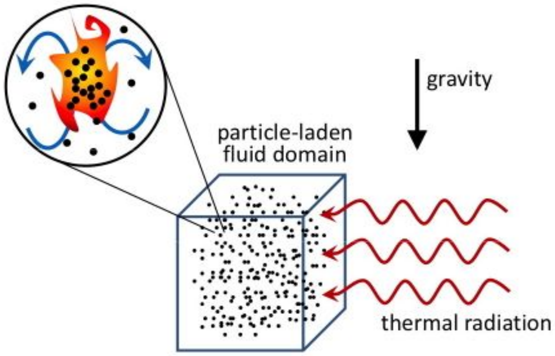
Clustering (preferential concentration)
in particle-laden turbulence - J. Eaton



Leverage experimental facilities to fully validate the simulations

Preliminary Computations

Can radiation generate and sustain turbulence in a particle-laden fluid?



Preliminary calculations carried out while writing the proposal!!!!

The "Simplified" Mathematical Model

CONTINUITY

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0$$

MOMENTUM EUQATION

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{1}{\mathrm{Re}}\frac{\partial \tau_{ij}}{\partial x_j} - \frac{\kappa}{N_p}\mathcal{P}(\frac{\mathcal{I}(u_i) - v_i}{\mathrm{St}})$$

ENERGY EQUATION

$$\frac{1}{\gamma}\frac{\partial}{\partial t}(\rho T) + \frac{\partial}{\partial x_j}(\rho T u_j) = \frac{1}{\mathrm{Re\,Pr}}\frac{\partial}{\partial x_j}(\frac{\partial T}{\partial x_j}) - \frac{2}{3}\frac{\kappa}{\mathrm{Pr\,St}N_p}\mathcal{P}(\mathcal{I}(T_g) - T_p)$$

LAGRANGIAN PARTICLE EQUATIONS

$$\frac{dx_i}{dt} = v_i \quad , \quad \frac{dv_i}{dt} = \frac{\mathcal{I}(u_i) - v_i}{\tau \tau_p} \quad , \quad \frac{dT_p}{dt} = \frac{\gamma\tilde{\alpha}}{\kappa\Gamma} + \frac{2}{3}\frac{\gamma}{\mathrm{Pr\,St}\Gamma}(\mathcal{I}(T_g) - T_p)$$

Dimensionless numbers

N_p

$$\gamma = \frac{C_p}{C_V}$$

$$\Gamma = \frac{C_{V\,p}}{C_V}$$

$$\mathrm{Pr} = \frac{C_p \mu}{k}$$

$$\mathrm{Re} = \frac{u_{ref} L_{ref} \rho_{ref}}{\mu}$$

$$\mathrm{St} = \frac{\tau_p u_{ref}}{L_{ref}} \qquad \tau_p = \frac{\rho_p d_p^2}{18\mu}$$

$$\kappa = \frac{N_p m_p}{L_{ref}^3 \rho_{ref}}$$

$$\tilde{\alpha} = \frac{\alpha N_p}{C_P L_{ref}^2 \rho_{ref} T_{ref} u_{ref}}$$

No buoyant forces - Lagrangian point particles (no interactions) -

Uniform radiation (Optically thin)

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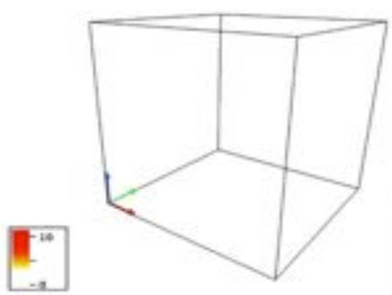
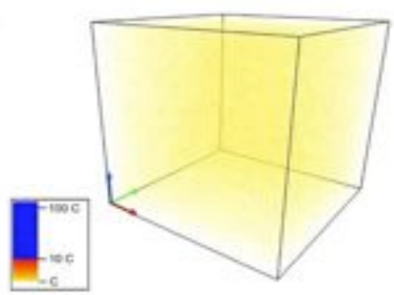
Preliminary Results

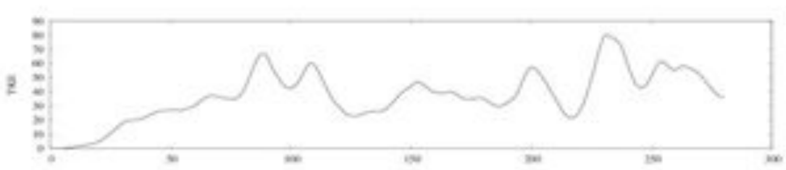
Effect of radiation on particle-laden free turbulence



Temperature



Particle Concentrations



Turbulent Kinetic Energy vs. time

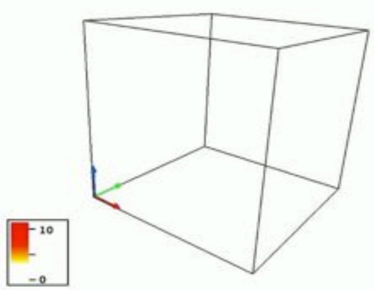
Small particle St #:
Absorbed radiation induces small temperature gradients and only weak turbulence

- R. Zamanski, H. Poraunsari & A. Mani

St = 0.018

Preliminary Results

Effect of radiation on particle-laden free turbulence



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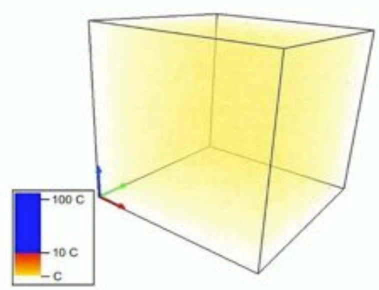

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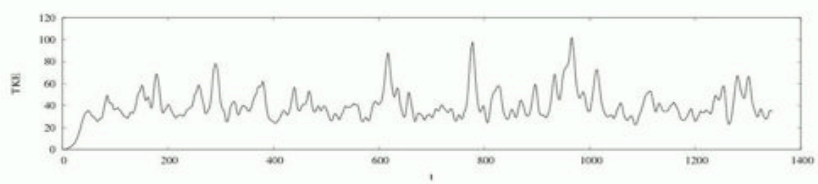


Turbulent Kinetic Energy vs. time

Large particles St #:
Absorbed radiation induces strong temperature gradients and particle clustering

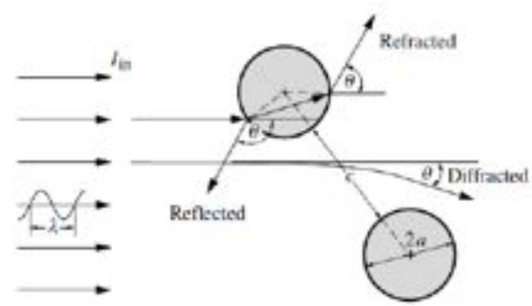
- R. Zamanski, H. Poraunsari & A. Mani

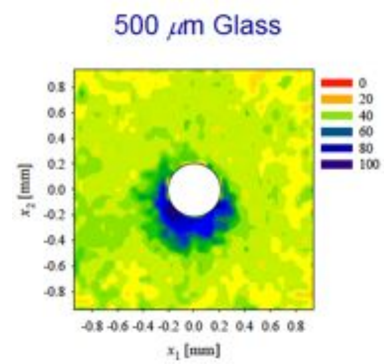
St = 0.35

Research Agenda, 1

Single-Physics Modeling

- Investigate radiation models
  - (in)homogeneous absorption
  - discrete ordinates
  - ray tracing
- Beyond point-particle tracking
  - finite-size effects
  - wall interactions, collisions



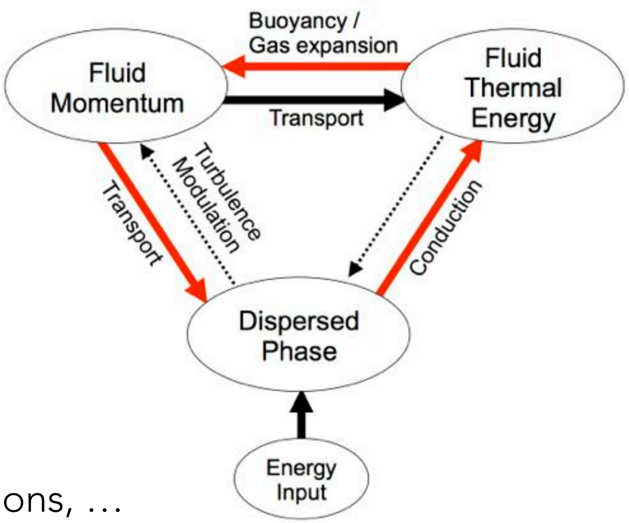


Tanaka & Eaton (2010)
Dissipation Measurements
via Micro-PIV

Research Agenda, 2

Coupling effects

- Radiation absorption by particles
  - Emissivity, surface properties
  - secondary absorption
- Heat transfer between particles & fluid
  - non-equilibrium
  - non-locality
- Turbulence
  - Modulaton by particles: dissipation in wakes, …
  - Radiation interactions with temperature/density fluctuations, …
- Three-way interactions



Regime of interest

Detailed measurements are limited….

Volume fraction (particle loading)

Ratio of T_{mix} and T_{source}

Shadow Fraction (opacity)

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ablative thermal protections	10^{-3}-10^{-1}		$7-30$	10^{-6}-10^{-4}		
Stanford experiment	0.5-10	10^4-10^5	≈ 0.1	10^{-5}-10^{-3}	0.1	0.1-1

Particle Stokes #

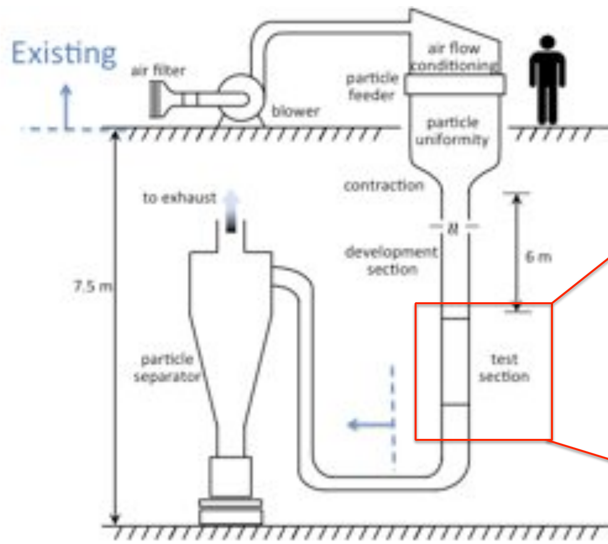
Fluid Re #

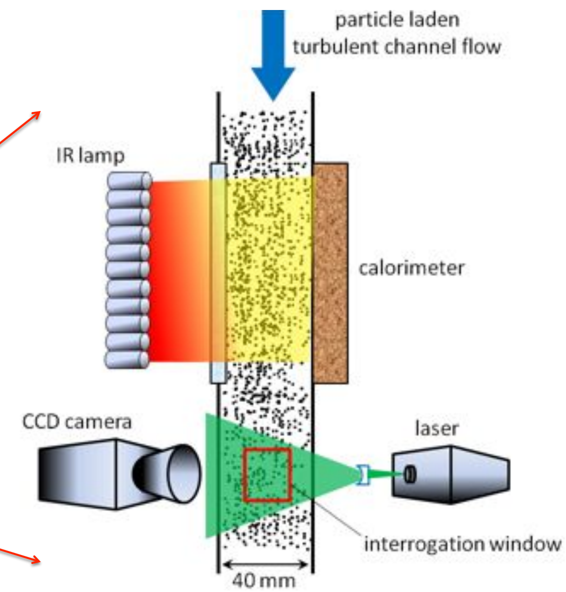
Fluid Ma #

Validation Experiment

Eaton vertical tunnel @ Stanford

- Re: 10K - 100K
- MLR: 0 - 50%
- Stokes #: 0.5 - 5
- Rad: 0 - 230kW/m^2
- ΔT_{max} : up to 300K





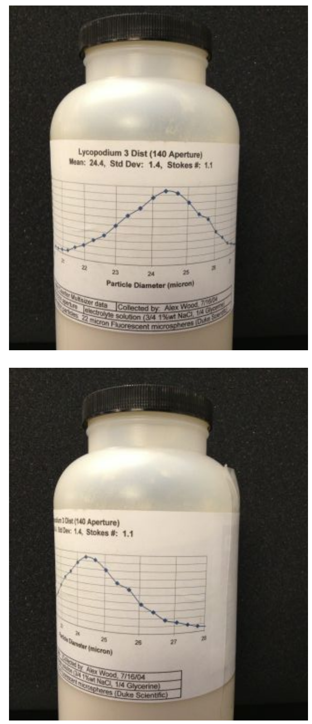
Uncertainty Quantification

Many sources of uncertainties

Naturally occurring
- Particle size/property variability
- Radiation forcing
- Losses through walls
- Inflow/Injection conditions

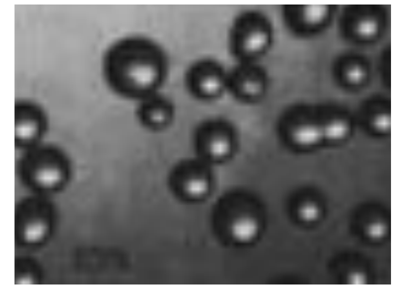
…

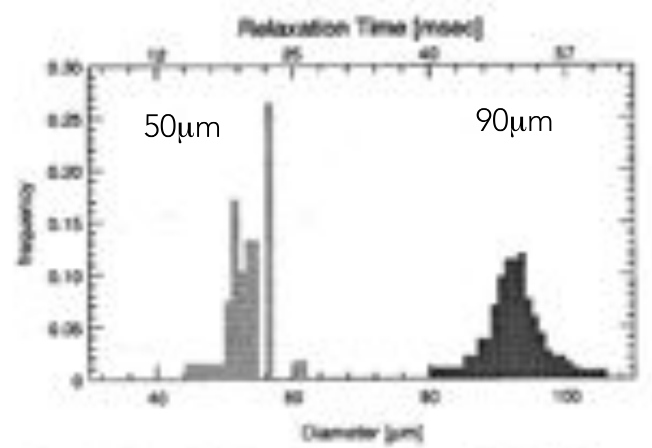
Mathematical models
- Particle physics
- Radiation/particle coupling
- Airflow/particle interactions
- …



Lycopodium (Eaton's Lab)

Sandia





Predictive Science Academic Alliance Program

Uncertainty Quantification

Leverage PSAAP UQLab

Algortihms for Aleatory UQ

- Stochastic expansion methods: beyond polynomials, e.g. Pade', wavelets
- Compressed sensing based sampling
- Key new elements: from random variables to random fields

Methodologies for Epistemic UQ

- Turbulence
- Key new element: model-form uncertainty influences the coupling

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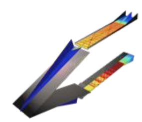
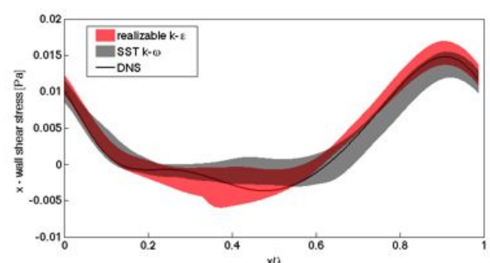
Methodologies for Epistemic UQ

- Turbulence
- Key new element: model-form uncertainty influences the coupling

Turbulence EUQ Approach

- Intrusive
- Non-probabilistic (no sampling) and accounts for model bias
- Includes physical constraints
- Provides insights into modeling errors
- Can be combined to "standard" aleatory UQ approaches with proper accounting





Gorle & Iaccarino POF 2013
Emory, Larsson, Iaccarino POF 2013

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UQ Research Plan

Turbulence

M1/M3 – Short term

- Extend PSAAP/EUQ approach (EUQ)

M3/M5 – Long term

- Develop intrusive stochastic subgrid velocity models (EUQ)

Particle Transport

M1-M3 – Short term

- Probabilistic particle size distribution
- Use SG/SC models (AUQ)

M2-M5 – Long term

- Increase # of uncertainties, e.g. particle shape, emissivity, etc. (AUQ)
- Spatially varying properties/random field model using physical constraints (EUQ)
- Incorporate stochastic subgrid velocity models (EUQ)

Radiation

M1 – Short term

- Probabilistic absorption coefficient

M2/M4 – Medium term

- Absorption coefficient as a random field
- Stochastic representation using KL or wavelet expansions
- Non-uniform input source

M3/M5 – Long term

- Stochastic discrete ordinance methods

Coupling

- Represent model-form EUQ of the interactions
- Keep track of the source for measuring relative importance

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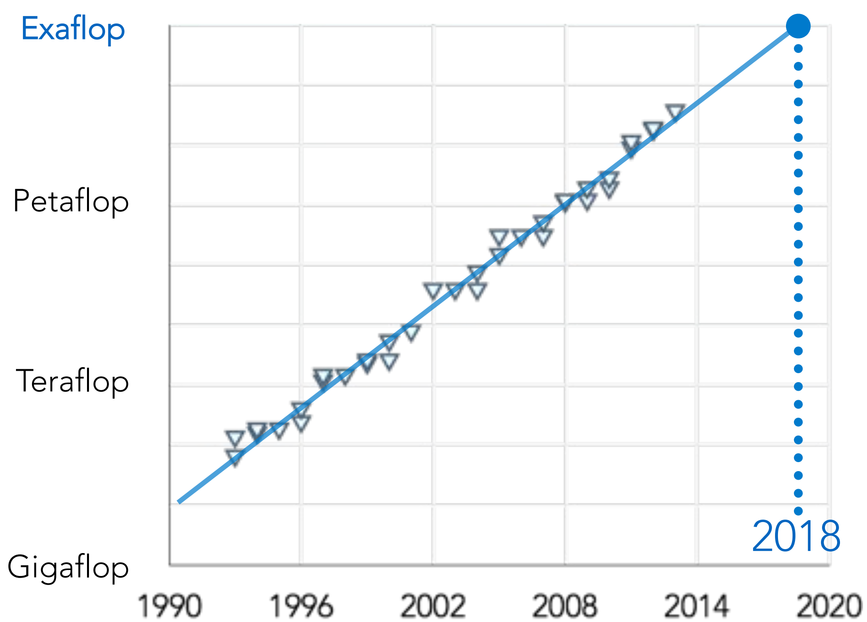
The road to exascale

How to exploit next-generation computational resources?



Complexity deriving from:

- Memory Hierarchies
- On-Chip vs In-Cabinet vs Across-System Communications
- Custom Non-conventional Networks
- Massive data management & mining
- Resiliency
- …

Software Abstractions

- CPU/GPU: C++, CUDA, OpenCL
- Queues for scheduling work between CPU/GPU?
- Nodes: Threads and locks – pthreads, OpenMP,…
- Cluster: Message passing – MPI
- …

Predictive Science Academic Alliance Program

The road to exascale

From **Teraflop** to **Petaflop** to Exaflop



The road to exascale

From **Teraflop** to **Petaflop** to Exaflop

The road to exascale…

Top systems display remarkable diversity

TOP500 JUNE 2013

	NAME	SPECS	SITE	COUNTRY	CORES	R_{MAX} PFLOP/S	POWER MW
1	**Tianhe-2 (Milkyway-2)**	NUDT, Intel Ivy Bridge (12C, 2.2 GHz) & Xeon Phi (57C, 1.1 GHz), Custom interconnect	NUDT	China	3,120,000	**33.9**	17.8
2	**Titan**	Cray XK7, Opteron 6274 (16C, 2.2 GHz) + Nvidia Kepler (14C, .732 GHz), Custom interconnect	DOE/SC/ORNL	USA	560,640	**17.6**	8.3
3	**Sequoia**	IBM BlueGene/Q, Power BQC (16C, 1.60 GHz), Custom interconnect	DOE/NNSA/LLNL	USA	1,572,864	**17.2**	7.9
4	**K computer**	Fujitsu SPARC64 VIIIfx (8C, 2.0GHz), Custom interconnect	RIKEN AICS	Japan	705,024	**10.5**	12.7
5	**Mira**	IBM BlueGene/Q, Power BQC (16C, 1.60 GHz), Custom interconnect	DOE/SC/ANL	USA	786,432	**8.16**	3.95

CPU Architecture **Accelerators**

BlueGene/Q

Cray XK7

Nvidia TESLA GPU

Intel Phi

What's next?

The road to exascale…

Not just performance…

Our multiphysics problem naturally involves diverse computational strategies

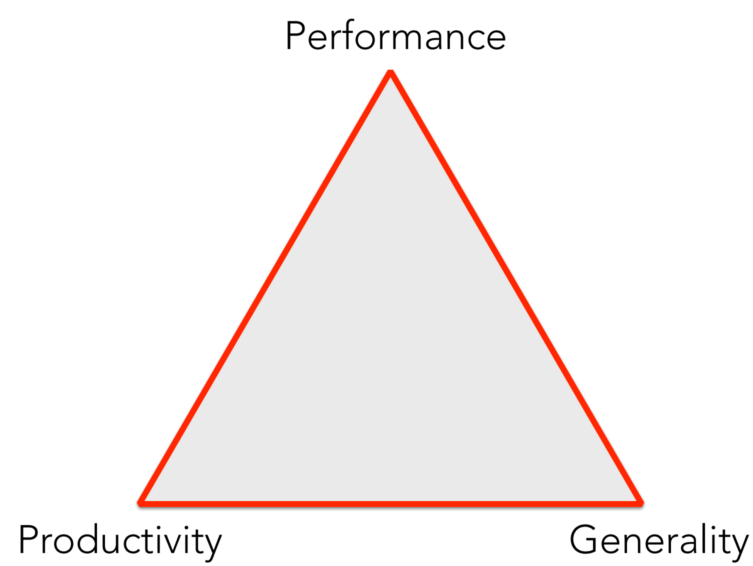
- PDE solvers (flow)
- Lagrangian tracking (particles)
- Integro-differential equation (radiation)

and several options

- Eulerian transport for particles
- Ray tracing for radiation
- ….

Key ingredients:

- Interoperable Domain Specific Languages
- Resiliency Libraries
- Legion Automatic Memory Mapping/Management



Predictive Science Academic Alliance Program

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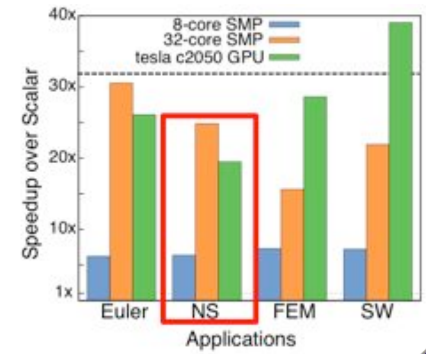
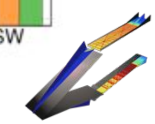
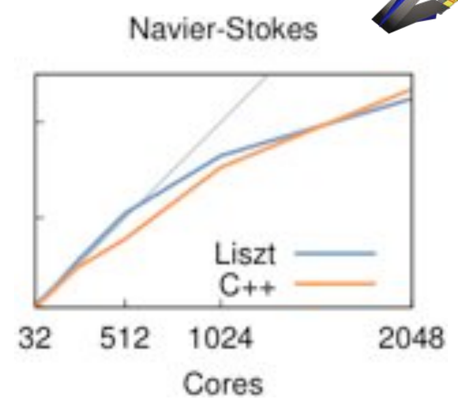






Predictive Science Academic Alliance Program

Software development

Where we are (framework from PSAAP):

- **Objectives** (*Why*):
  - Ensure Quality of software through V&V (unit/system/regression testing)
  - Ease and enhance experience of:
    - Developers: enable & promote <u>collaboration</u> (modularity + automation)
    - Users: seamless cross-platform installation & execution
- **Drivers** (conceptual *How*):
  - Apply principles of Continuous Integration
  - Incorporate best-practices from Open-Source community
- Implementation (practical *How*): combine git, gitolite, cgit, CMake, CDash, Redmine, rsnapshot, cron, MediaWiki, Doxygen, …

Framework encapsulates code through <u>weak coupling</u>

Predictive Science Academic Alliance Program

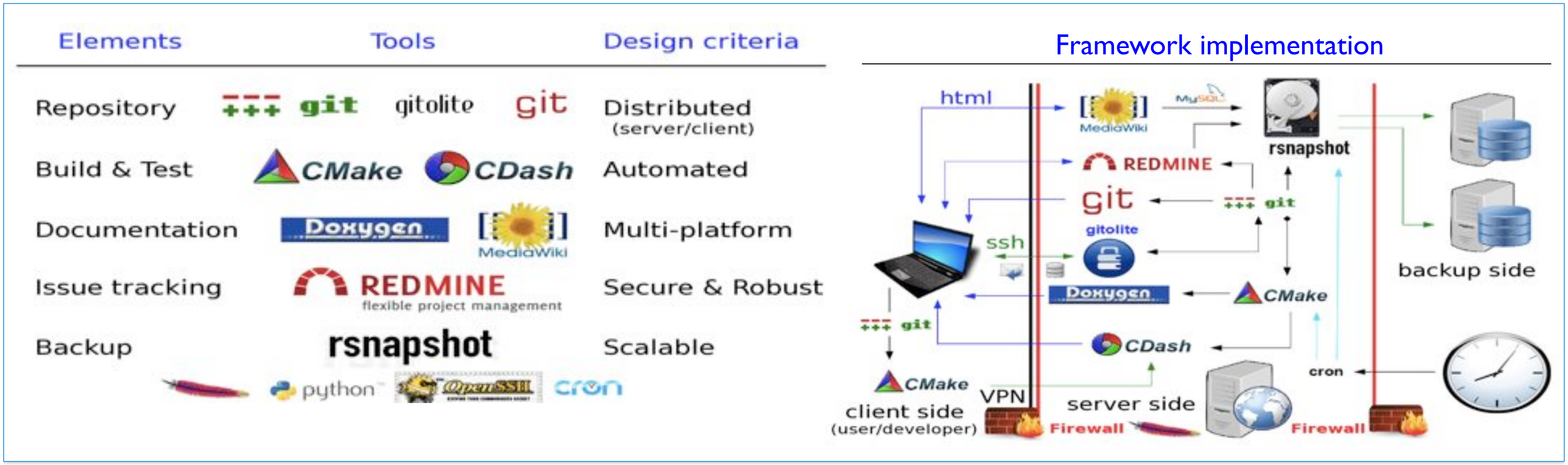
Software development

Elements	Tools	Design criteria
Repository	git gitolite git	Distributed (server/client)
Build & Test	CMake CDash	Automated
Documentation	Doxygen MediaWiki	Multi-platform
Issue tracking	REDMINE flexible project management	Secure & Robust
Backup	rsnapshot	Scalable
	python OpenSSH cron	

- **Implementation** (practical *How*): combine git, gitolite, cgit, CMake, CDash, Redmine, rsnapshot, cron, MediaWiki, Doxygen, …

Framework encapsulates code through <u>weak coupling</u>

Software development



- **Implementation** (practical *How*): combine git, gitolite, cgit, CMake, CDash, Redmine, rsnapshot, cron, MediaWiki, Doxygen, …

Framework encapsulates code through <u>weak coupling</u>

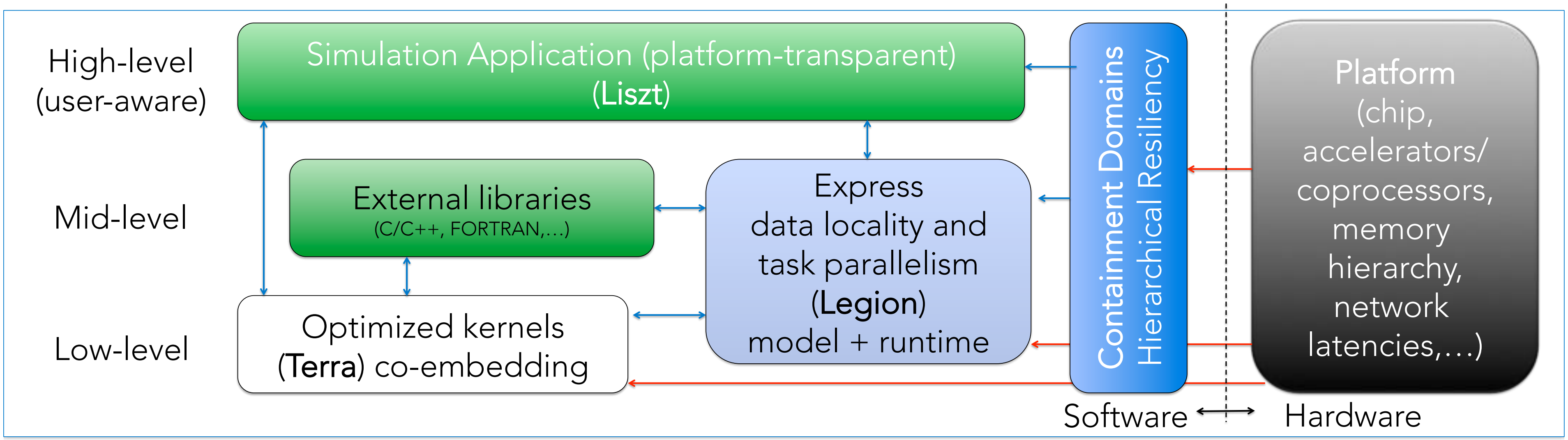
Software development – in PSAAPII

- **Objectives** (*Why*):
  - develop programming model & framework that
  - enable V&V+R(eliable) scientific simulations at **exa** scale and
  - ensure **transparency** and **accessibility** for non-experts in HPC

- **Drivers** (conceptual *How*):
  - Bridge **Computational** & **Computer** Science (models & algorithms/systems)
  - Integrate:
    - High-level, natural application-targeted programming
    - Mid/low-level platform-aware parallelism models and runtime systems

- **Implementation** (practical *How*):
  - Write application in **Liszt** domain-specific language (*high-level* abstraction)
  - Express logical-region locality and task parallelism in **Legion** (*mid/low-level*)
  - Co-embed in **Terra** to exploit high-performance optimization (*low-level*)
  - Interface **Containment Domains** for hierarchical fault-tolerance/resiliency

Software development – in PSAAPII



- **Implementation** (practical *How*):
  - –Write application in Liszt domain-specific language (*high-level* abstraction)
  - –Express logical-region locality and task parallelism in Legion (*mid/low-level*)
  - –Co-embed in Terra to exploit high-performance optimization (*low-level*)
  - –Interface Containment Domains for hierarchical fault-tolerance/resiliency

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PSAAP II

Project organization and research team…

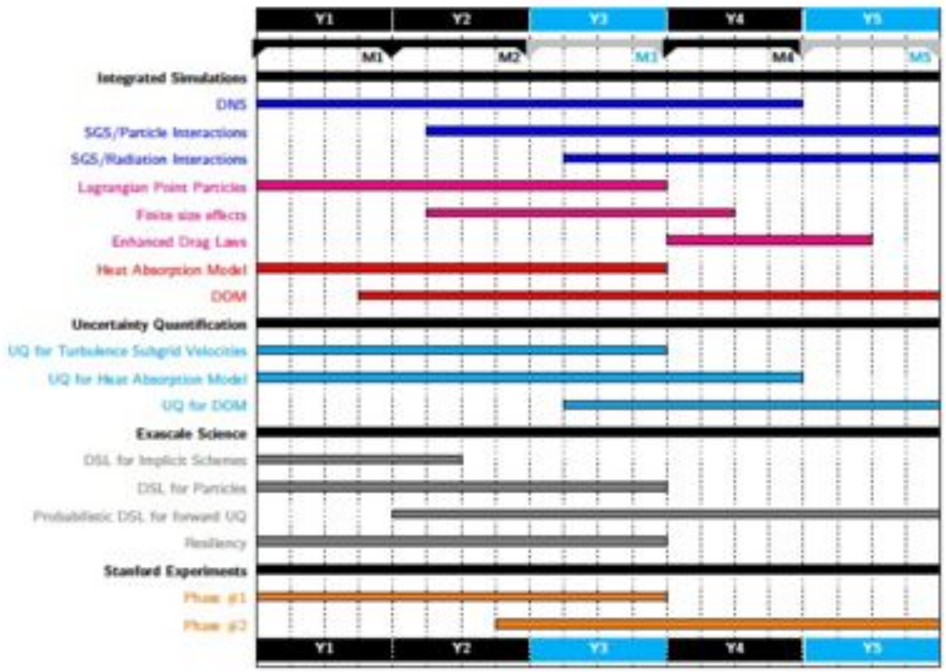
PSAAP II Research Team

Aiken	Boyd	Glimm	Mahesh	Doostan	Erez
Alonso					
Darve					
Eaton					
Hanrahan					
Iaccarino					
Lele					
Mani					
Moin					
Papanicolaou					

PSAAP II Research Team

CS	Aiken	Boyd	Glimm	Mahesh	Doostan	Erez
CS/Physics	Alonso	Physics (radiation)	UQ	Physics (particles)	UQ	CS (resiliency)
CS	Darve					
Physics	Eaton					
CS/Physics	Hanrahan					
UQ/Physics	Iaccarino					
Physics	Lele					
Physics	Mani					
Physics	Moin					
UQ/Physics	Papanicolaou					

PSAAP II Project Plan



M1 Predictive simulations of low-Reynolds number turbulence with low mass loading under a moderate radiation input. Radiation is modeled using a lumped heat absorption model. Direct comparisons to Stanford's experiments will be carried out. Uncertainties account for the effect of imprecision in the specification of the boundary conditions and the parameters used in the absorption model. The current PSAAP codes, enhanced with Lagrangian tracking and the radiation model will be used.

M2 The objective in Year 2 is to increase the scope of the M1-type simulations by considering a more realistic uncertainty model for the absorption coefficient used in the radiation transport; a random field model will be considered. This will naturally require an increased number of computations; to enable these investigations, a DSL-enhanced version of the code will be deployed.

M3 In Year 3, the computational tools developed in the previous years will be exercised within a comprehensive UQ study. The objective is to investigate the effect of uncertainties in both the radiation source uniformity and particle size. In addition, the effect of the model uncertainty in the absorption model will be characterized and the resulting mixing efficiency variability will be characterized in detail. In this context the problem requires multiple M2-type simulations, further increasing the overall computational complexity.

M4 The objective in Year 4 is to perform simulations in a range of controlling parameters different from that considered in M1. Increases in the Reynolds number, the particle loading and a more realistic representation of finite-size effects in the particle transport will be considered. The use of resiliency libraries will be demonstrated.

M5 The goal in Year 5 is to revisit the UQ assessment carried out in Year 3 in the regime corresponding to the M4-type simulations. In addition to all the previous uncertainties, we will also consider additional sources related to the properties of the particles, for example emissivity imperfections. This will considerably enhance the computational complexity because of the increased dimensionality in the representation of the uncertainty. We anticipate to leverage the development in a probabilistic DSL to enable these final simulations.

PSAAP II – First steps

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  - Administrative & financial structure in place
  - Website and intranet launched (90% complete)
- Introductory Town Hall Seminars (4 held)
  - Background information
  - Review of the state of the art
- Research meetings (weekly)
  - Discussion of proposed activities and challenges
  - Task Planning
- Research activities
  - design of the P-code
  - (very) preliminary computations
- Personnel
  - Senior research associates (1 down, 1 to go)
  - First group of PhD students (4 out of 6 are US citizens)

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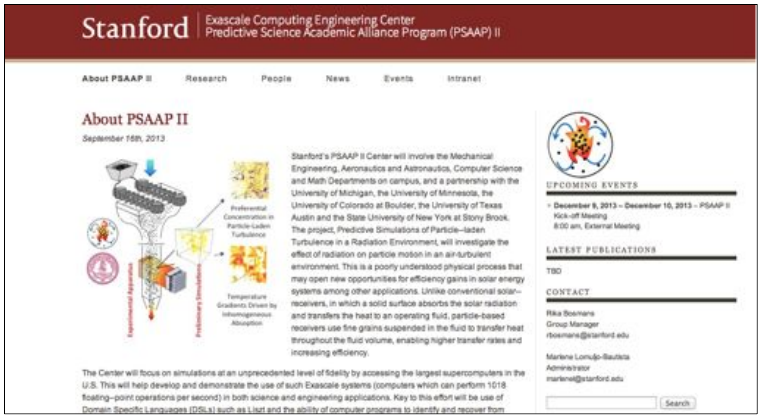

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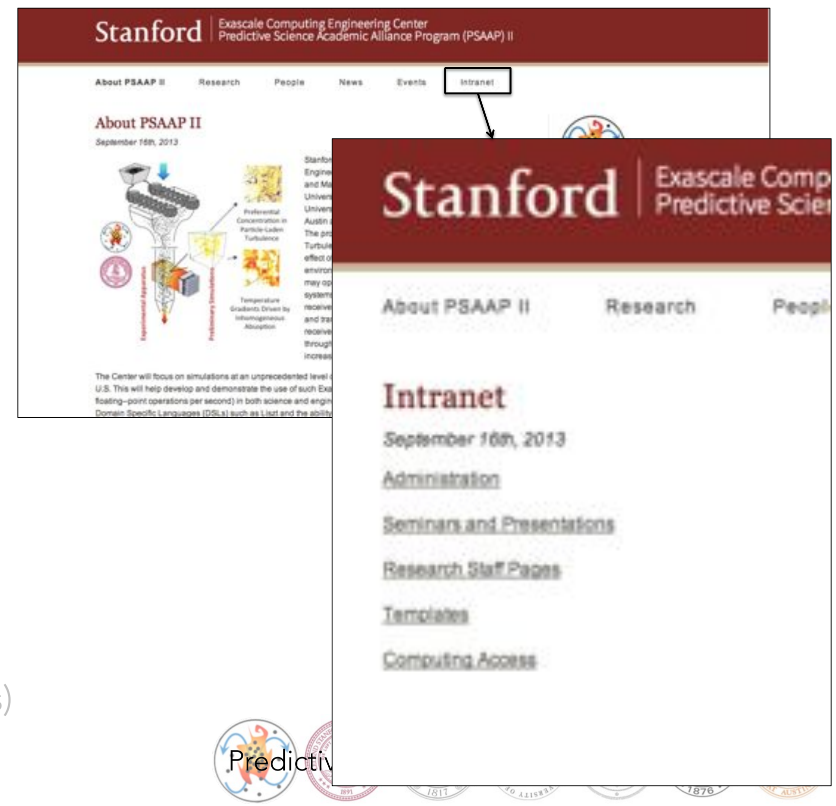

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Prof. Ali Mani
"Interactions of particle transport, turbulence and radiation, what do we know?" 9/20/2013
Prof. John Eaton
"Preferential concentration in particle-laden turbulence" 9/27/2013
Prof. Iain Boyd (Michigan)
"Modeling radiat
Prof. Pat Hanrahan
"DSL and Legion

[youtube channel]

Predictive Science Academic Alliance Program

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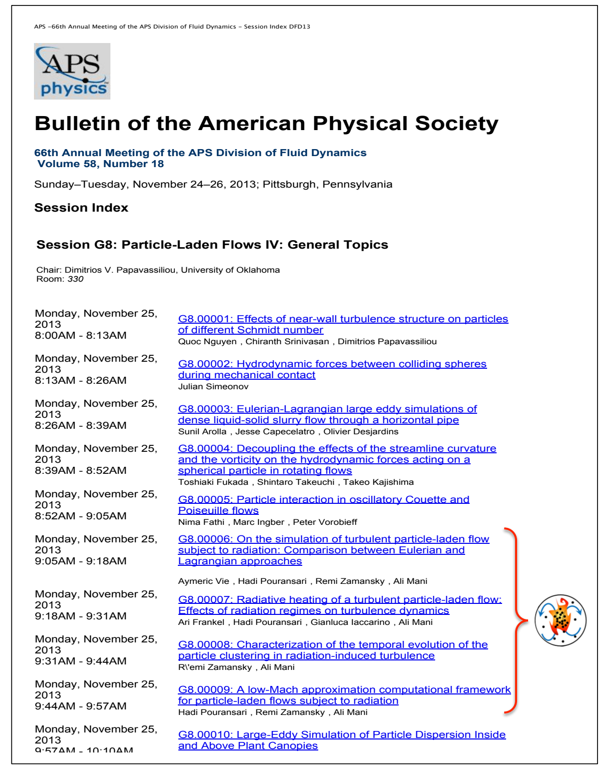

APS -66th Annual Meeting of the APS Division of Fluid Dynamics - Session Index DFD13

APS physics

Bulletin of the American Physical Society

66th Annual Meeting of the APS Division of Fluid Dynamics
Volume 58, Number 18

Sunday–Tuesday, November 24–26, 2013; Pittsburgh, Pennsylvania

Session Index

Session G8: Particle-Laden Flows IV: General Topics

Chair: Dimitrios V. Papavassiliou, University of Oklahoma
Room: *330*

Monday, November 25, 2013 8:00AM - 8:13AM	G8.00001: Effects of near-wall turbulence structure on particles of different Schmidt number Quoc Nguyen , Chiranth Srinivasan , Dimitrios Papavassiliou
Monday, November 25, 2013 8:13AM - 8:26AM	G8.00002: Hydrodynamic forces between colliding spheres during mechanical contact Julian Simeonov
Monday, November 25, 2013 8:26AM - 8:39AM	G8.00003: Eulerian-Lagrangian large eddy simulations of dense liquid-solid slurry flow through a horizontal pipe Sunil Arolla , Jesse Capecelatro , Olivier Desjardins
Monday, November 25, 2013 8:39AM - 8:52AM	G8.00004: Decoupling the effects of the streamline curvature and the vorticity on the hydrodynamic forces acting on a spherical particle in rotating flows Toshiaki Fukada , Shintaro Takeuchi , Takeo Kajishima
Monday, November 25, 2013 8:52AM - 9:05AM	G8.00005: Particle interaction in oscillatory Couette and Poiseuille flows Nima Fathi , Marc Ingber , Peter Vorobieff
Monday, November 25, 2013 9:05AM - 9:18AM	G8.00006: On the simulation of turbulent particle-laden flow subject to radiation: Comparison between Eulerian and Lagrangian approaches Aymeric Vie , Hadi Pouransari , Remi Zamansky , Ali Mani
Monday, November 25, 2013 9:18AM - 9:31AM	G8.00007: Radiative heating of a turbulent particle-laden flow: Effects of radiation regimes on turbulence dynamics Ari Frankel , Hadi Pouransari , Gianluca Iaccarino , Ali Mani
Monday, November 25, 2013 9:31AM - 9:44AM	G8.00008: Characterization of the temporal evolution of the particle clustering in radiation-induced turbulence R\'emi Zamansky , Ali Mani
Monday, November 25, 2013 9:44AM - 9:57AM	G8.00009: A low-Mach approximation computational framework for particle-laden flows subject to radiation Hadi Pouransari , Remi Zamansky , Ali Mani
Monday, November 25, 2013 9:57AM - 10:10AM	G8.00010: Large-Eddy Simulation of Particle Dispersion Inside and Above Plant Canopies

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In conclusion

Many scientific challanges…

- Physics: three-way coupling of turbulence/particles/radiation is largely unexplored; *is there a self-sustaining cycle? Is the interaction robust across difference regimes?*
- SQA: each physics components has a favorite numerical method; *how to combine in a single, efficient and verifiable framework?*
- Exascale: DSLs have been demonstrated for single-physics problems; *can we combine multiple, interoperable DSLs and manage data efficiently and reliably on hybrid architectures?*
- UQ: aleatory and epistemic uncertainties are abundant and of different origin: *can we embed UQ techniques in the software infrastructure? Can we use advances in stochastic sensing techniques to speed up the UQ assessment?*
- Validation: modern and detailed measurements are scarce; *can we design a controlled apparatus with large parameter variation to validate our tools?*

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a collaboration between

Stanford University - University of Michigan - Stony Brook University
University of Minnesota - University of Colorado - University of Texas